1,3-Dimethyl-4-ethylbenzene 874-41-9 | DTXSID0061246

Model Performance

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N	Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 3.89 days

Global applicability domain: Inside

Local applicability domain index: 8.24e-01

Confidence level: 8.82e-01

Nearest Neighbors from the Training Set

Image not found

1,3-Dimethyl-4-ethylbenzene

Measured: 24.3 Predicted: 3.89

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2-Ethyl-p-xylene Measured: 12.5 Predicted: 3.70

Image not found

1-Ethyl-2,3-dimethylbenzene

Measured: 61.9 Predicted: 4.15

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1-Ethyl-2-methylbenzene

Measured: 24.3 Predicted: 3.88

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3-Ethyltoluene Measured: 12.5 Predicted: 3.26